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Equation of State Modeling: Lowering Barriers to Progress

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- Constitutive relations are input for simulations
  Essential for predictive capability
  Higher resolution increases need for accuracy
  Example: HE & detonation waves
  meso-scale simulations of hotspot ignition
- EOS modeling is mature field
  A lot is known
  Engineering details are important
  Too much for any individual
  Need cooperative approach
- Technology available for closer cooperation
  Every researcher has dedicated workstation
  and connected to internet
  Share resources beyond journal articles
  Data and source code require standards
  Need consensus on format or language
  Any interest ?

Barriers to Progress

- Getting models from literature to applications

  Large effort to implement and debug new model

  - Details are often vague or sketchy
  - Special tricks for robustness

- Calibration of parameters

  Hand-crafted procedures

  Too labor intensive

  - Need to be automated

- Documentation & Validation

  Is the domain specified ?

  Are uncertainties in data specified ?

  Calibration procedure specified ?

  Is sensitivity of model parameters specified ?

  Comparison with other experiments and models ?

- How much effort would it be to reproduce ?
- Or to incorporate new experimental data ?

  - Calibration is non-linear fit
  - Constraints: monotonicity & convexity

  Complete EOS requires potential: e, F, G or H

  - Need at least two derivatives

Current practice is <u>too inefficient</u>

- Duplication of effort
- Difficult to transfer improvements between codes

  Different EOS data structures and IO

  Lack of common tools

  Always short on manpower

- Difficult to reproduce results
- Difficult to compare models

  Data files in different formats or not available

  Lack of automation

  Codes not portable

  <u>Leads to low standards</u>

- Progress is slow

  Individuals starting from scratch

  rather than building on work of others

  and continually improving models

<u>Need to share resources</u>

Both information and tools

Take advantage of internet

Requires some standardization

<u>Interchangeable components</u>

Common software tools

Focus on EOS package as an example

Design goals

- Treat different EOS models in uniform manner
  Enable different application to use exact same EOS
  Separate application from details of model
- Provide thermodynamic functions
  pressure, temperature, sound speed, etc.
- Provide high level functions
  Isentropes, shock loci, etc.
- Modular and flexible
  Easy to add new materials
  Easy to add new models
- Allow for proprietary or classified data
  Clean separation of general purpose and proprietary
- Extendible to other constitutive properties
- Portability

Type of EOS models

1. Sesame tables

   Closest 'model' to standard

      EOSpack interface (not always used)

   Piece together models for wide range

      smoothness, monotonicity & convexity constraints

      table resolution & interpolation

2. Analytic models

   Thermodynamically consistent

      Ideal gas, stiffened gas, van der Waal

   Incomplete EOS (limited domain of phase space)

      Mie-Grüneisen, JWL, BKW, etc.

3. Semi-analytic models

   Solve implicit equation

   Examples:

      P & T equilibrium for mixture

      Equilibrium porous EOS

Best choice for particular application ?

Depends on <u>region of phase space</u> of interest

Model Development

- Build on existing models

  Simple mixture rules

  pressure and temperature equilibrium

  Alloy

  mixed cell EOS for Eulerian algorithm

  Solid + Liquid

  Melt curve from matching Gibbs free energy

  Explosive

  Reactants + products

  Detonation Hugoniot as well as shock Hugoniot

- Testing of new models

  Check for consistency

  For example, compare sound speed

  from analytic formula

  with generic finite difference routine

  Compare with data & other models

  Isotherms, Hugoniots, specific heats, etc.

Hydro Applications

More capabilities then evaluating pressure & sound speed

- Design & Analyse experiments
  Lead waves & impedance matches
  Same material models as in simulations
- Simplify input
  Material names rather than specifying parameters
  Set initial state based on (P, T) or (V, e)
  Set state as point on Hugoniot
- Boundary conditions
- Loss of resolution & robustness issues
  Example, resolving discontinuities
    Impact problems resolved using Riemann solver
    Isentropes for centered rarefactions

Structure of EOS package

- Database

  Model parameters for materials

  Number and meaning differ

  Issue of validation & quality control

  Account for units

- Application Interface

  Defines an EOS structure

  Pointers to thermodynamic functions

  pressure, temperature, sound speed, etc

  Higher level functions for useful quantities

  Isotherms, Isentropes, Hugoniots etc.

  Solution to impedance match problems

- Low level routines

  Fittings forms for different models

  Initialization for specific model

  Shared objects to implement particular models

  Dynamically linked library

  Enables package to be easily extended

- Natural extension

  Server for database and shared objects

Usage

1. Initialize database

   Specify name of file(s)

   Package reads database

2. Fetch EOS *handle* for each material

   Call database function with name of material

   Package loads needed library

   and initializes EOS with parameters from database

3. Evaluate thermodynamic quantities

   Through function calls, *e.g.*,

   `pressure(handle,V,e)`

Trade-off

Treat all materials in same manner

Level of indirectness

Package is extendible

- To add new material of known type

  Add parameters to database file

- To add new EOS type

  Generate shared object with low level routines

  Then add parameters to database file

  No need to recompiling application

Software Engineering

Example of what can be done for hydro interface

EOS plugin for James Quirk's AMRITA

http://t14web.lanl.gov/Staff/rsm/preprints.html#EOSpackage

http://t14web.lanl.gov/Staff/rsm/preprints.html#EOSlib

- Parser for input

Purpose is to translate input
from form that is convenient for user
to form that code can easily handle

Setup for impedance match test problem

```
utilize EOS

set mat1 = EqPorous::estane
set mat2 = Hayes::HMX
set Ps   = 3.1

def SolutionField
    getstate on right hugoniot($mat1) at P=$Ps  -> W'left
    getmaterial $mat2  -> W'right
    setfield W'left  X[] <  $Nc
    setfield W'right X[] >= $Nc
end def
```

Advantages of input parser

- Convenient and Less error prone

  Material by name

      code fetches parameters from database

  Point on Hugoniot

      code computes hydro state

- Facilitates automation

  Clearer and easier to change

  Programmable interface is more flexible

      Problem specific setup not hard wired

- Long lived input files

  Parser is interface

  Can change implementation of hydro code

  Same input file for different codes

Scripting language

Needs to be well thought out

Flexible and concise for common idioms

- Parser for output

Comparison with theory

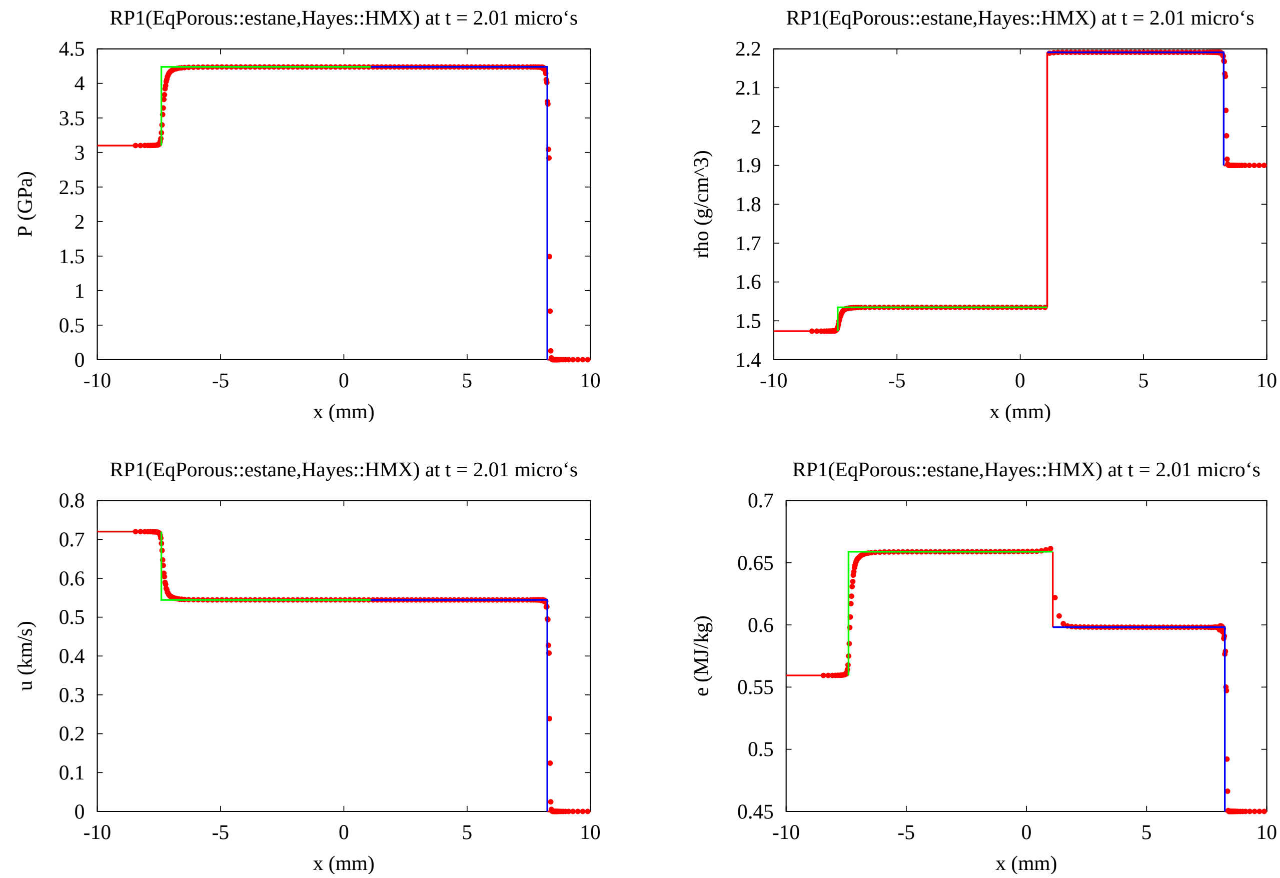
```
solve RiemannProblem(left_state, right_state) -> $label
OneDPlot {
  variable  = $V[]
  xoffset  #= -$Nc*$dx + $time*$left_u
  file_data = $label/$V.data
}
ProfileRiemannSolution {
   handle    = $label
   var       = $V
   t         = $time
   x_l      #= -$Nc*$dx
   x_r      #=  $Nc*$dx
   dir       = .
   plot      = "$V.data" with points lt 1 pt 7 ps 1
}
```

Scripts facilitates reusable capabilities

`OneDPlot` to pick out numerical profile

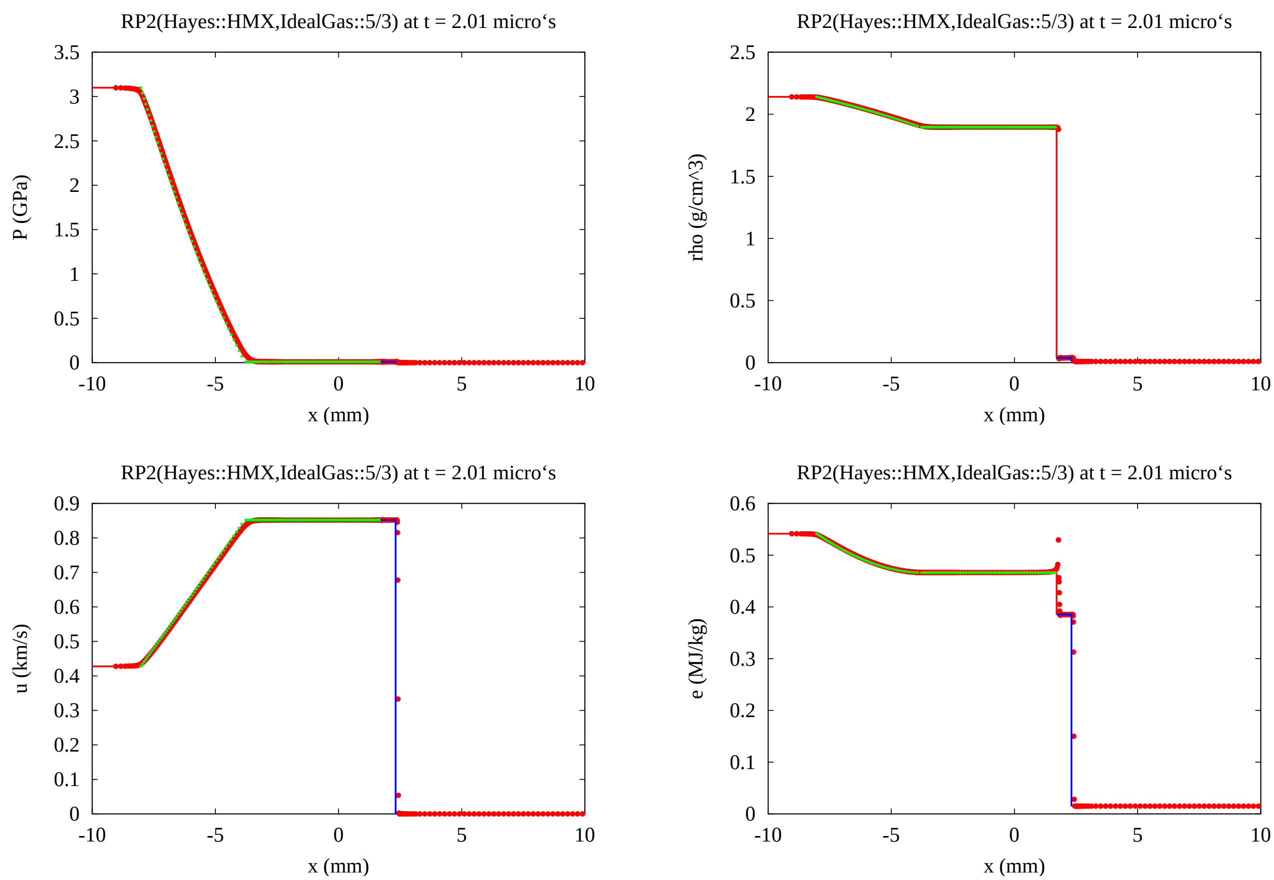
`ProfileRiemannSolution` to generate theoretical profile

Case I: Two outgoing shocks



Comparison of numerical profiles and exact solution.

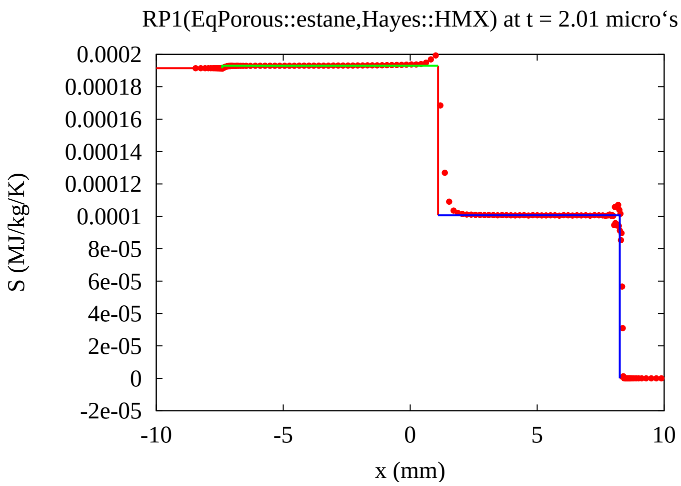
Case II: Reflected rarefaction and transmitted shock



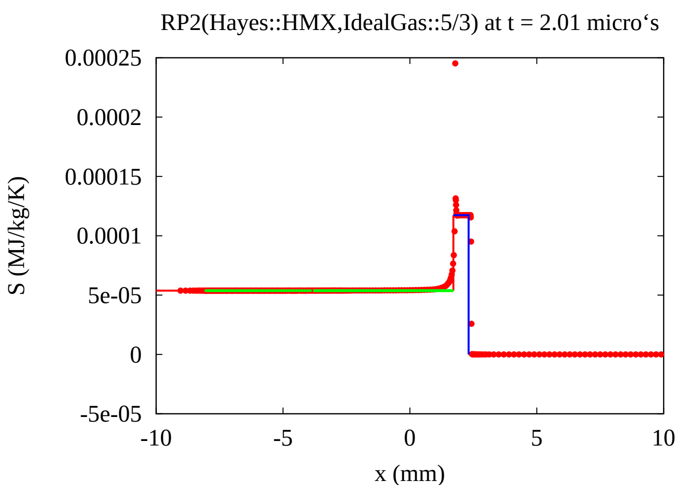
Comparison of numerical profiles and exact solution.

Entropy Error

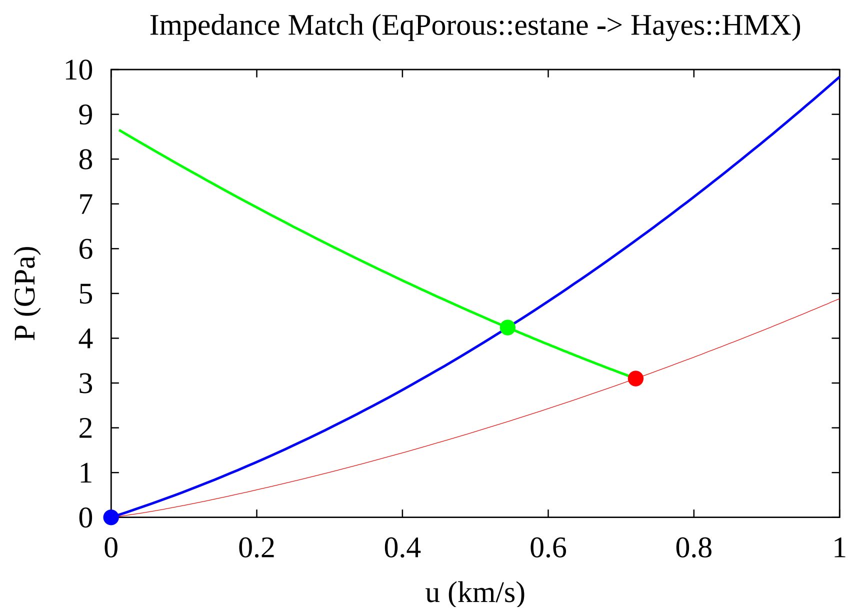
Case I

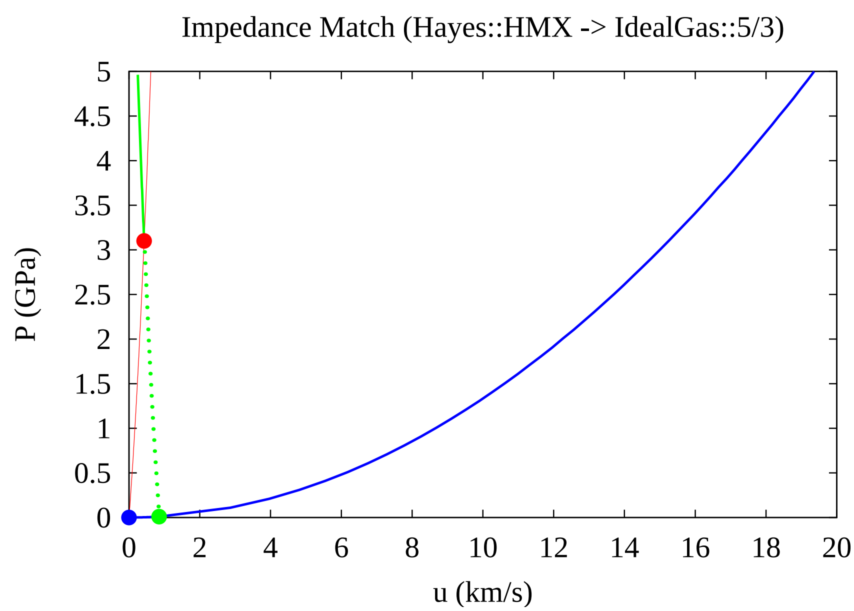


Case II



Wave Curves for Impedance Match Problems





Methodology

Long run — more efficient and easier for user

- Build-up library of script subroutines
  re-usable and programmable
  worthwhile to expend extra effort to do job well
- Simple idioms for common patterns of work
  Less labor intensive
    automated rather than hand crafted
  Allows for more thorough and systematic studies
    sensitivity studies to assess uncertainties
- Consistency
  Same EOS routines to design experiments,
    simulate results and analyze data.
- Comparing models
  Vary only model or only hydro algorithm
  Plot results on same scale or overlay two cases

To use new techniques effectively
requires different style

Present style is too labor intensive
Need to take advantage of computer power
to automate and run simulations

Cooperative Approach

- Common language or protocol

  Interchangeable components

  Specialized language tailored to hydro applications

  - Facilitates sharing of simulated results

  Reproducibility, Comparisons & Portability

  - Language should outlive the hardware

- Social issues

  All models have strengths and weakness

  Journal articles tend to lack balance

  - Skewed to advantages of new model
  - Driven in part by funding

  More extensive testing of models is necessary

  - Models need to be readily accessible
  - Possible with internet

  Mutually beneficial to share resources

- Reward system

  Sharing code only worthwhile if

  - Software well crafted
  - Documentation is provided

  Software engineering

  - Needs to be recognized and encouraged